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Title: Introduction to RF-Structures and Their Design Chapter 4: Numerical

Design Tools

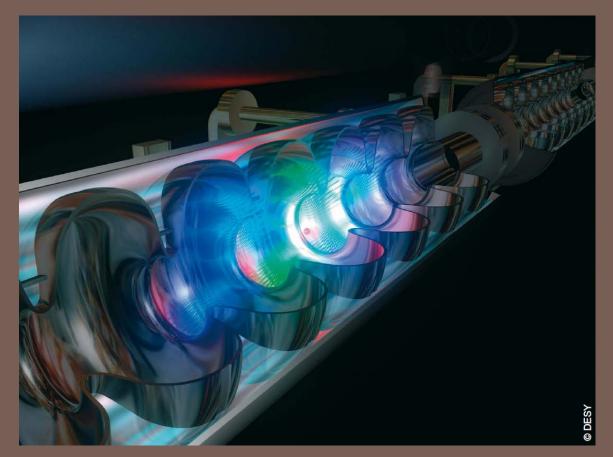
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INTRODUCTION TO RF-STRUCTURES AND THEIR DESIGN – CHAPTER 4 NUMERICAL DESIGN TOOLS

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AOT-HPE, June 2012

Abstract

Introduction to RF-Structures and Their Design Chapter 4: Numerical Design Tools Frank L. Krawczyk LANL, AOT-AE

The numerical design chapter of the class addresses two topics: (1) Numerical Methods that include resonator design basics, introduction to Finite Difference, Finite Element and other methods, and (2) Introduction to Simulation Software that covers 2D and 3D software tools and their applicability, concepts for problem descriptions, interaction with particles, couplers, mechanical and thermal design, and finally a list of tips, tricks and challenges.

4th week

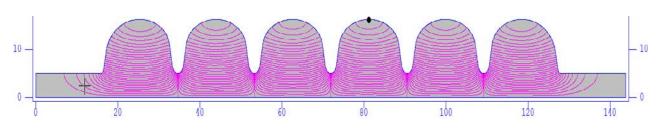
- □ Design Tools (4. week)
 - Numerical Methods
 - Resonator design basics
 - Basics of Finite Difference and Finite Element Methods
 - Other methods
 - Software
 - 2D software
 - 3D software
 - General concepts of problem descriptions
 - Interaction with particles, couplers, mechanical and thermal design
 - Tips, tricks and challenges

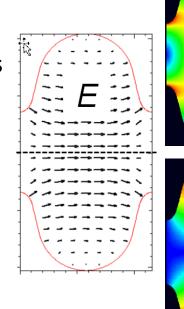
Design Basics

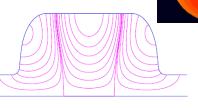
- There is a huge number of numerical design tools available addressing a wide range of methods and needs
- RF-structures with few exceptions cannot be designed analytically
- The design task: obtain a geometry that can contain or transport electro-magnetic (EM) fields with specific properties
- Beyond the basic EM properties, designs might consider secondary properties and additional conditions (mechanical, thermal, interaction with charged particles)

- Design Basics
 - Design of resonating structures
 - Pill-box/Elliptical resonators
 - Quarter and half-wave resonators
 - RF-gun cavities
 - Waveguides
 - Mathematical problem: Solution of Maxwell's Equations
 - for eigenvalues and eigenvectors (Helmholtz)
 - for a time-harmonic drive (Helmholtz)
 - fully time-dependent (Faraday & Ampere's Law)

- Relevant properties primary, direct result of the simulation
 - Cavity eigenmode frequencies
 - Electric & magnetic field patterns of modes
 - Acceleration mode
 - Higher order modes (HOM) deflecting,
 specific mode band, "full" spectrum
 - Peak surface fields (electric and magnetic)
 - Peak surface field locations
 - Waveguides: propagation constant



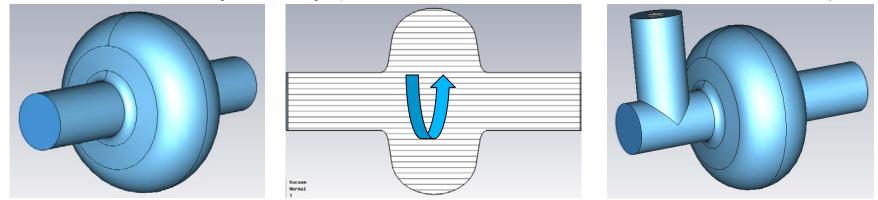




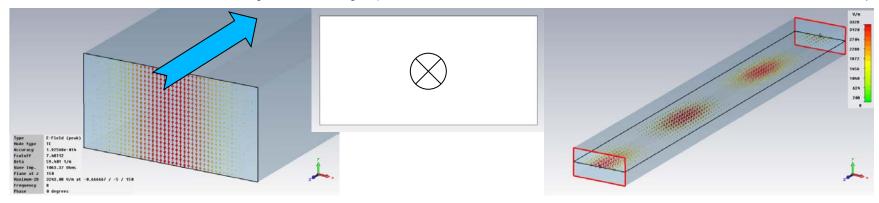
- Relevant properties secondary, require postprocessing steps based on the primary results
 - Resonator losses P_c
 - Resonator loss distribution
 - \square Quality factor Q= ω U/P_c
 - Accelerating voltage ~ E*g
 - Transit time factor T
 - Shunt Impedance $(V*T)^2/P_c$
 - Coupling properties (cell-to-cell or to coupler)

- The selection of design software needs to consider the simulation results you are aiming for
 - Type of structure
 - Symmetries
 - Materials involved
 - Details of rf-properties needed
 - Interaction with other structures (e.g. couplers)
 - Interaction with other physics characteristics
 - Mechanical, Thermal, Static Fields, Particles

- Selection of calculation domain (2D vs. 3D)
 - Azimuthal symmetry (for structure + restrictions for solutions)



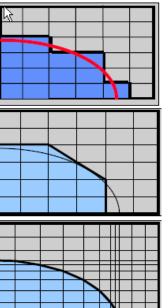
■ Translational symmetry (for structure + restrictions for solutions)

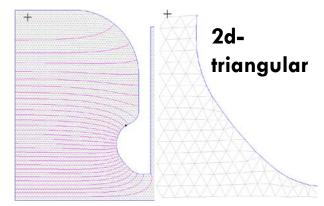


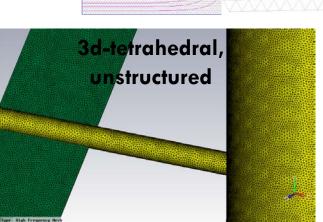
 Discretization of the calculation domain: Cartesian, triangular, tetrahedral, regular or unstructured grid,

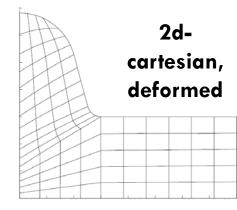
sub-gridding

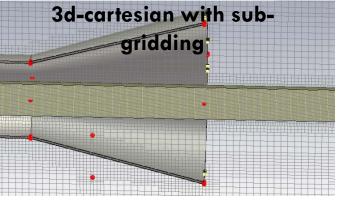
Quality of representation





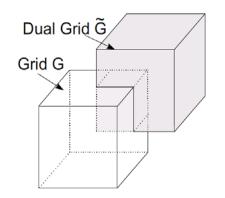


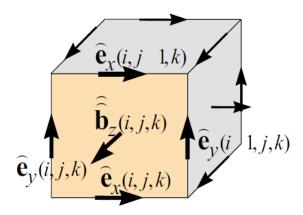




- Formulation of Maxwell's equations in discrete space
- Continuous equations will be translated into matrix equations that are solved numerically
- Methods vary in
 - Discretization of space
 - Discretization of field functions
 - Consideration of surfaces, volumina, solution space, exclusion areas
 - Roles of boundaries
 - Locations of the allocation of solutions: points, edges, volumina
 - Applicable numerical methods
 - Support of modern computer architectures (vector, parallel, multi-core, ...)

- Finite Difference (FD) or Finite Integration (FIT):
 - Differential or integral operators are replaced by difference operators
 - Equations couple values in neighboring grid elements
 - □ → often regular elements, sparse banded matrices
 - quality of surface approximations depends on software implementation
 - Allocation of the fields in the discrete space (YEE algorithm)





Differential operators

1st derivative

2nd derivative

$$\left(\frac{\partial u}{\partial x}\right)_i \approx \frac{u_{i+1} - u_i}{\Delta x}$$
 forward difference
$$\left(\frac{\partial u}{\partial x}\right)_i \approx \frac{u_{i-1} - u_{i-1}}{\Delta x}$$
 backward difference
$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2} + \mathcal{O}(\Delta x)^2$$

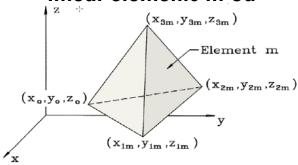
$$\left(\frac{\partial u}{\partial x}\right)_i \approx \frac{u_{i+1} - u_{i-1}}{2\Delta x}$$
 central difference

- Coupling between elements provided by common points
- Coefficients include material properties along edges/surfaces
- Solutions minimize local energy integral in each cell
- □ Special FIT properties: difference operators fulfill discrete vector-analytic operators (e.g. curl grad $\equiv 0, ...$)

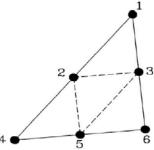
□ Finite Elements (FE):

- Differential or integral operators act on discrete approximations of the field functions (base polynomials of low order)
- □ → regular or irregular elements, banded matrices, sparseness depends on element type
- mostly superior surface representation

Representation of field with linear elements in 3d



Representation of field with second order elements in 2d



$$\mathbf{E}_m = \alpha_{1m}\mathbf{x} + \alpha_{2m}\mathbf{y} + \alpha_{3m}\mathbf{z}. \quad \phi(x,y) = a_0 + a_1x + a_2y + a_3x^2 + a_4xy + a_5y^2.$$

- Coupling between elements provided by common points
- Coefficients include material properties along edges/surfaces
- Solutions minimize global energy integral in calculation volume
- Increased order reduces number of required elements for a given accuracy, but might reduce sparseness of matrices
- Suggested Reading:
 - FD: Allan Taflove, Susan Hagness, Computational Electrodynamics: The Finite Difference Time Domain Method, 3rd Edition (2005)
 - FIT: Thomas Weiland, Marcus Clemens:

 http://www.ipier.org/PIER/pier32/03.00080103.clemens.p

 df
 - FEM: Stan Humphries:
 http://www.fieldp.com/femethods.html

- Other Methods
 - Boundary Integral Methods or Method of Moments: Continuous volume solutions from sources in discretized metal surfaces
 - Transmission Line Matrix: Solving resonator problems as lumped circuit models
 - Scattering Matrix Approaches: Quasi optical approach based on diffraction from small features
 - Specialized solvers for fields inside conductors (metals/plasmas)
 - Specialized solvers merging optical systems with regular RFstructures (e.g. Smith-Purcell gratings)

Software Tools - 2D

- The Superfish family of codes (http://laacg.lanl.gov/laacg/services/)
 - 2d (rz, xy), FD, triangular, TM (TE), losses, post-processing, part of general purpose suite
- The Superlans codes (D.G.Myakishev, V.P.Yakovlev, Budker INP, 630090 Novosibirsk, Russia)
 - 2d (rz, xy), FE, quadrilateral, TM, losses, post-processing
- The codes from Field Precision (http://www.fieldp.com/)
 - 2d (rz, xy), FE, triangular, TM/TE, losses, some postprocessing, part of general purpose suite

Software Tools - 2D

- 2D modules of MAFIA (or even older versions like URMEL, TBCI, ...)
 - 2d (rz, xy), FIT, Cartesian, TM/TE, losses, post-processing, general purposes suite, PIC and wakes
 - these are not distributed anymore, but still used at accelerator laboratories
- While 2D codes were the standard up to 10 years ago, their use is decreasing. Their strength is speed and accuracy. One strong reason for those codes is the design of SRF elliptical resonators, where peak surface fields are of importance.

Software Tools - 3D

- □ MAFIA (http://www.cst.com/)
 - 2d/3d (xy, rf, xyz, rfz), FIT, Cartesian, losses, post-processing, general purpose suite, PIC & wakes
 - Historically, MAFIA was the first 3d general purpose package for design of accelerator structures
- □ GdfidL (http://www.gdfidl.de/)
 - 3d (xyz), FIT, Cartesian, losses, post-processing, general purpose suite, wakes, HPC support
- CST Microwave Studio (http://www.cst.com/)
 - 3d (xyz), FIT/FE, Cartesian/tetrahedral, losses, post-processing, general purpose suite, PIC &wakes, thermal, HPC support
- □ HFSS (http://www.ansoft.com/products/hf/hfss/)
 - 3d (xyz), FE, tetrahedral, losses, post-processing, general purpose suite, interface to mechanical/thermal, HPC support

Software Tools - 3D

- Analyst
 - (http://web.awrcorp.com/Usa/Products/Analyst-3D-FEM-EM-Technology/)
 - 3d (xyz), FE, tetrahedral, losses, post-processing, HPC support, wakes
- □ Comsol (http://www.comsol.com/)
 - 3d (xyz), FE, tetrahedral, losses, post-processing, part of a multiphysics suite including mechanical/thermal and beyond
- Vorpal (http://www.txcorp.com/products/VORPAL/)
 - 3d (xyz), FE, tetrahedral, losses, post-processing, particles & wakes,
 HPC support
- □ Remcom Codes (http://www.remcom.com/)
 - 3d (xyz), FD, Cartesian, losses, post-processing, HPC support

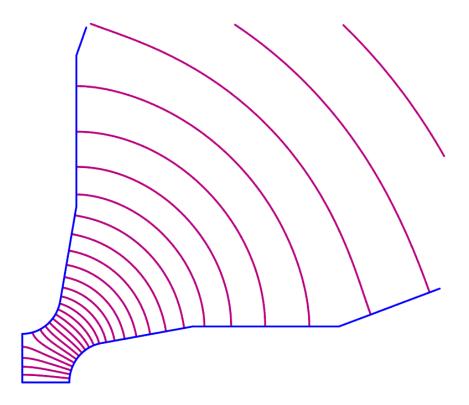
Software Tools - 3D

- SLAC ACE3P
 - (http://www.slac.stanford.edu/grp/acd/ace3p.html)
 - 3d (xyz), FE, tetrahedral, losses, post-processing, PIC & wakes, HPC support
- The strengths of 3D codes
 - Treatment of complex geometries
 - Support of general CAD formats
 - Flexible post-processing
 - Professional interfaces and design controls but they are slower and need much more expensive resources
- □ Links to more software
 - http://emclab.mst.edu/csoft.html
 - http://www.cvel.clemson.edu/modeling/EMAG/csoft.html

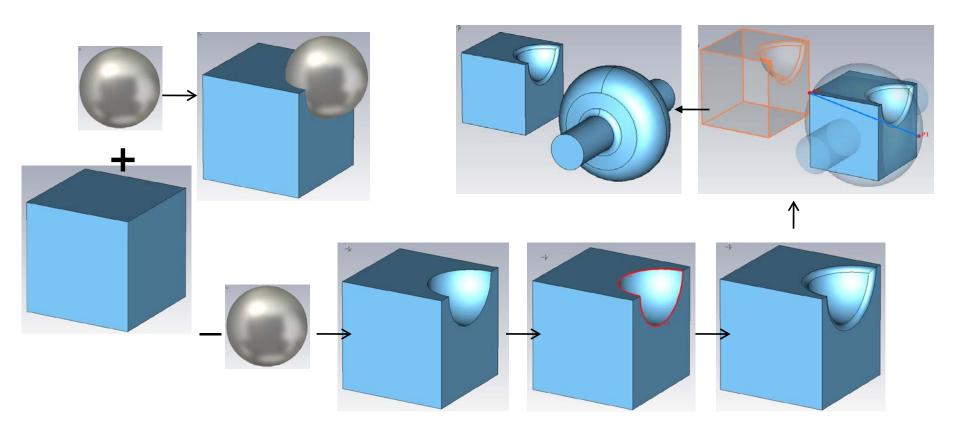
Resonator geometry

2d: polygons describe contours, straight-forward for linear segments, cumbersome for curved polygons, most codes do not allow use of parameters

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3d: assembly of primitives with Boolean superposition, CAD style tools that allow definition of separate sub assemblies, import/export of CAD models, blends, extrusions,



Material properties

- For RF-properties only the interior of resonators needs to be modeled
- In general the outside space will be assigned the properties of the metallic enclosure
- Enclosing metals only required for thermal/mechanical considerations, for a mix of metals, or for internal features
- Dielectric or permeable inclusions, like rf-windows, ferrites, ... will need to be added
- Perfect conductors and non-lossy dielectrics standard
- Newer codes also allow permeable and lossy properties
- Few rf-codes handle non-linear materials (except for magnetostatics codes)

Material properties

- Losses in dielectrics and ferrites need to be considered during the resonator evaluation. They require appropriate complex solvers
- Treatment of losses in metals is a special case
 - For rf-resonators loss-considerations do not need modeling of the skin-depth layer of the metal
 - Explicit consideration of losses is handled by the modeling software
 - For most codes it is suggested to assume perfect conducting metals for the field solutions (does not require complex solvers). The rf-losses are calculated in a post-processing step from the bulk resistivity and the surface magnetic fields

Boundary conditions

- PDE solutions require specifications of solutions at the volume boundaries. For the solution of Maxwell's Equations the conditions are given by the physical problem. Common conditions are
 - Dirichlet: Constant potential or vanishing tangential field
 - Neumann: Constant potential derivative or vanishing normal field
 - Mixed: combined Dirichlet and Neumann conditions (uncommon)
- In (often) rectangular calculation volumes, boundary conditions on each surface can be chosen to be different
- For the definition one needs to be aware, if the specification is for the electric or magnetic field properties on the boundary

Boundary conditions

- Waveguide ports: Waveguides connected to resonators can be modeled by short longitudinally invariant sections. Their terminations are modeled as an impedance-matched layer. This boundary condition is important for evaluation of resonator -coupler interaction
- Open boundaries: Simulation of solutions radiating into open space. The methods depend on the physics problem. Methods used are solutions expansions, absorbing boundary conditions, or Perfectly Matched Layers (PML), an improved type of absorbing condition less prone to frequency or angle of incidence

- Besides the descriptions relevant to the rf-structure, there is a number parameters that need to be set before a simulation can be performed. These include
 - Problem-type
 - Meshing controls
 - Frequency estimate (for meshing or for time-harmonic solvers)
 - Some beam properties (for transit-time factors and other secondary properties, for parametric generators of special geometries like elliptical resonators)
 - Solver type and configurations, ...

Software Tools – More Features

- <u>Parameterization</u>: flexible description of geometries allows for better design strategies and optimization (most 3D codes)
- Optimization: User defined goals and strategies can be defined in many 3d suites, some support in 2d
- Post-processing: All codes listed support basic postprocessing in the form of solution display and calculation of secondary quantities relevant to accelerator applications. Some 3d-suites allow additional user-defined post-processing
- Parallel software: The need for larger resources led to the addition of solvers that support massively parallel computations (multi-core, MPI, GPUs)

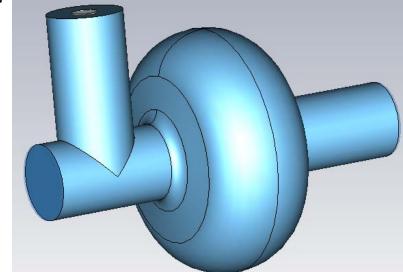
Interaction with Couplers

- Basic resonator design: ideal structures, ignore power feeds, vacuum pumping and couplers. Historically, this originates from the limitations of 2d codes
- Some 3d codes support waveguide ports, allow to model coupling to a matched load or drive from a matched source
- Driving a high-Q resonator with a source impractical, as number of rf-cycles ~ to Q required to drive the fields into steady state

□ Important use of these features: calculation of Q_{ext} or calculation of

mode loading due to an HOM coupler

 Combining solutions from calculations with Dirichlet and Neumann conditions (Kroll-Yu or Balleyguier) achieve the same with larger effort



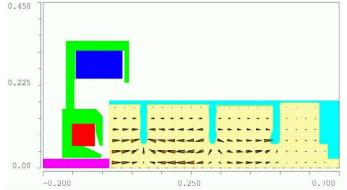
Field Interaction with Particles

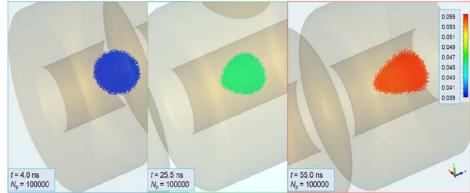
Beam Dynamics input

EM fields are often used for beam-dynamics simulations, some codes export directly in suitable formats (e.g. Superfish for Parmela, Impact, Opal). Often free ASCI export for conversion to other input formats is supported

Particle tracking

Some code suites support electron emission from surfaces for the design of particle guns (photo injectors or thermionic guns). Those emissions are for well-defined timings and distributions (different from field emission or multipacting effects). Typically those simulations require electro- and magnetostatic fields in conjunction with rf-fields.





Field Interaction with Particles

Wakefields

- Charged particle bunches crossing a metallic enclosure (constituting a change in cross-section) generate electromagnetic fields (wakefields) that can act on itself, on following bunches (geometric wakes) or for very short bunches can generate unwanted heating on rf-surfaces (even in smooth pipes) or in secondary components (resistive wakes).
- While there are very good specialized codes for this, some general purpose codes add such excitations (in the time-domain, 2d and 3d) for comprehensive structure evaluation including the potential for beam disruptions.

The particle bunches are modeled as rigid lines line charges (Gaussian or user-defined) – no self-consistent calculations

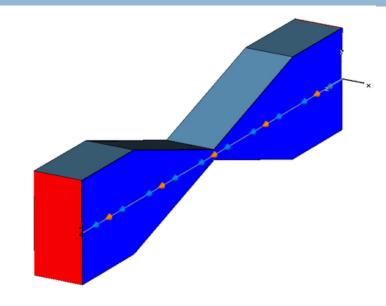
■ Wake fields are combinations of HOMs in a resonator. If HOMs are calculated, their action on a beam can also be calculated from the mode properties ($k_{loss} = \omega/4 * R/Q$)

More on Wakefields - Software

- □ ABCI: http://abci.kek.jp/abci.htm
- □ ECHO 2D: Zagarodnov, DESY
- □ RWBBU: Nakamura, Univ. of Tokyo
- MAFIA-T2: former TBCI, CST
- MAFIA-T3: CST
- CST Particle Studio:

More on Wakefields - Categories

Geometric wakes

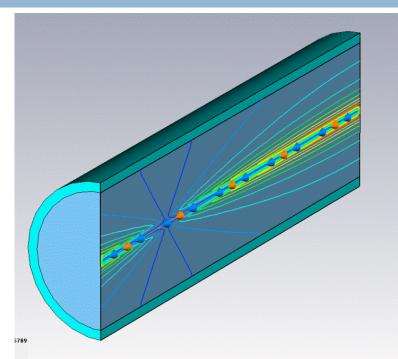


- Intra-bunch effects: effect from the beam on to bunch itself
- Multi-bunch effects: For a train of bunches succeeding bunches might see wakes from earlier bunches
- Re-circulation: If fields damp very slow, effects can be seen on succeeding paths (ring or ERL)

More on Wakefields - Categories

Resistive wakes

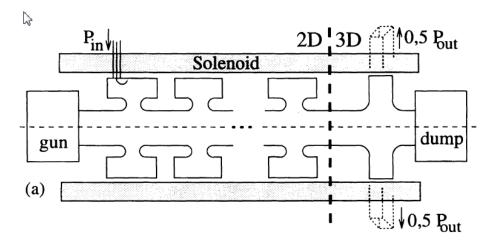
- Result in
 - pipe heating and
 - □ increase of longitudinal and transverse emittances

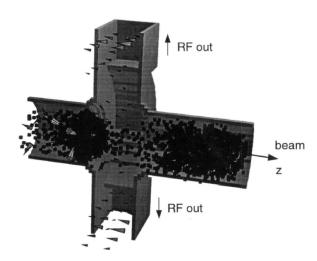


Field Interaction with Particles

Particle-In-Cell (PIC)

- When field actions back onto the particles cannot be ignored, particle-in-cell algorithms are needed to solve particle motions and field developments self-consistently. Some codes support these computationally very intensive calculations. This adds design of power generators (like klystrons) to the code capabilities.
- These simulations i.g. require a combination of static electric and magnetic fields in conjunction with rf-fields





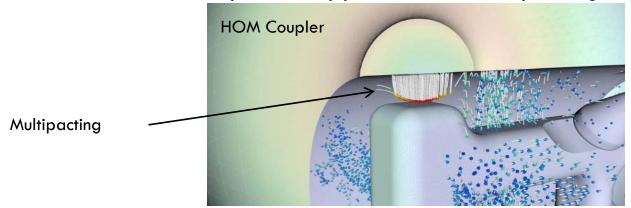
Field Interaction with Particles

Multipacting and Field-emission

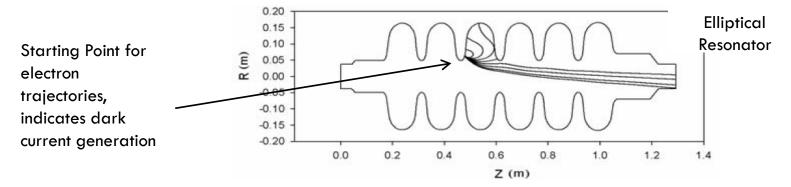
- Spontaneous creation of surface electrons due to surface electric fields can be an issue for proper operation of resonators.
- Field-emission (non-resonant) limits performance of superconducting resonators for high field gradients. Multipacting (resonant) in addition can damage structure surfaces.
- While there is little support for spontaneously emitted electrons, some codes allow systematic studies of trajectories of electrons emitted in different surface regions with a range of emission energies.
- Consideration of secondary emission yields indicates the potential for multipacting problems

Field Interaction with Particles

- Multipacting and Field-emission
 - MWS, ACE3P & Vorpal do support full 3D multipacting simulations



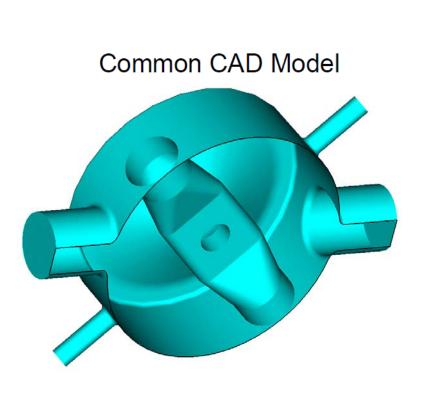
 A wrapper named FishPact uses Superfish as mesh and field generator for multipacting simulations

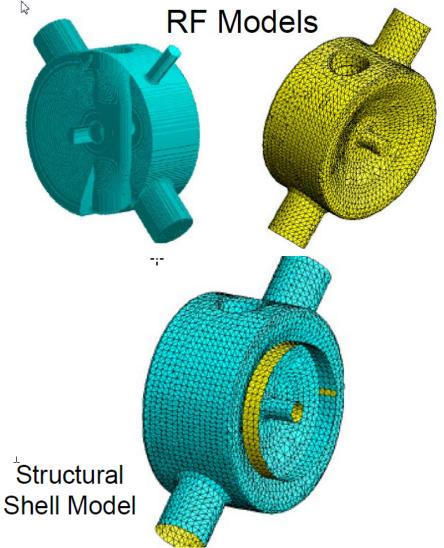


Interaction with Mechanical/Thermal Design

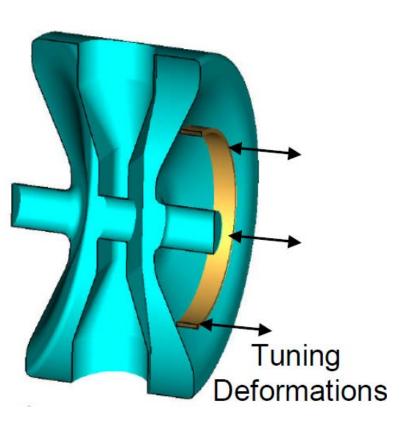
- RF-designs are not stand-alone, feasibility of fabrication, mechanical stability and thermal loads needs to be considered also
- General purpose and multi-physics tools permit evaluation of several aspects without a complete re-build for each domain of evaluation
- Note however: EM fields require meshing of enclosed volume, thermal/mechanical properties require meshing of enclosure, this needs to be considered during the structure generation
- Effects due to mechanical deformations are small, one needs to pay attention that effects are real and not driven by discretization errors

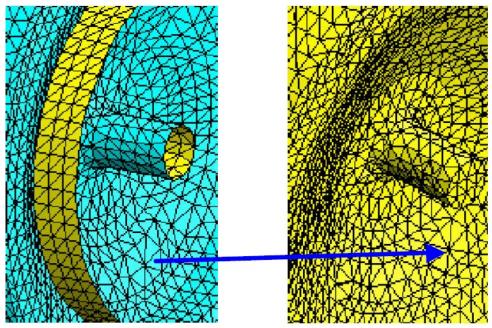
Interaction with Mechanical/Thermal Design





Interaction with Mechanical/Thermal Design





Shell Mesh ← → Volume Mesh
Common nodes allow recalculation
of RF-case without re-meshing
(reduces discretization error)

Numerical Challenges

- Feature rich software is mostly full 3D, which makes structure development slow. Where 2D would not suffice – consider parallel versions
 - Several of the 3D codes support solver versions on high performance computing platforms.
 - The minimum support is for multiple cores in standard cpus.
 - There are also versions for clusters (using mpi) or for using GPUs.
 - Analyst, ACE3P, Vorpal are predominantly written for HPC platforms

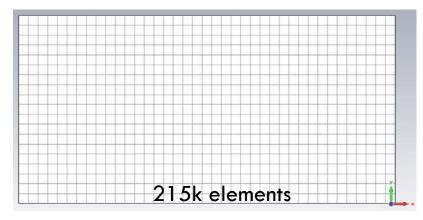
Numerical Challenges

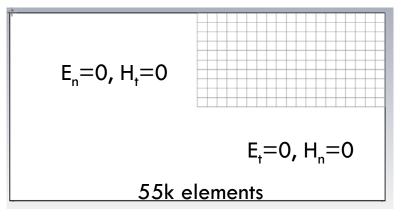
- Overall property calculations are reliable, some 3D codes have problems for peak surface fields. This is related to
 - Surface representation quality
 - Eigenvalue solvers solve the Helmholtz Equation only in E or H and construct the complimentary solution from Maxwell's Equations (large amplitude fields might result from small amplitude complimentary field, or vice versa)
- Use 2d when very accurate solutions are needed
- Do verification with changes in meshing
- Problems are also caused by "changes in topology"

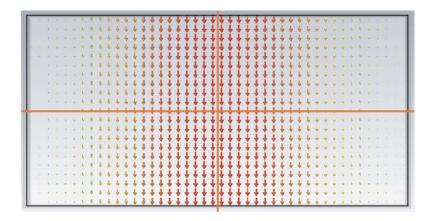
Peak fields "jump" when outlines cross

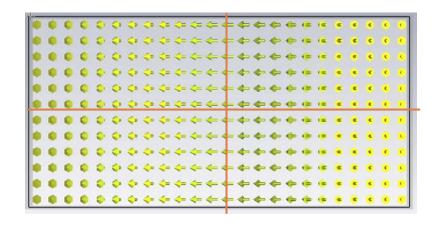


<u>Use of symmetries:</u> Boundary conditions cannot only be used to define the properties at the outside of a problem. The can also be used to reduce problem size or enforce finding specific modes









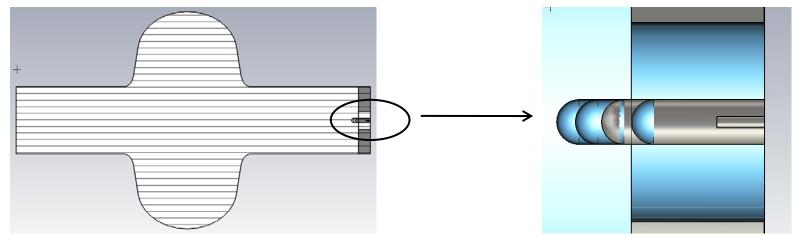
- SRF-structures often requires modeling of resonators with open beam-pipes. Standard boundary conditions are only approximately correct. Open boundaries are often not supported for eigenvalue solvers. To estimate, if a beampipe is long enough to not affect the solution, the following approach is suggested:
 - Calculate twice, once with Dirichlet and once with Neumann conditions. The change in frequency should be very small
 - Add a metal (flange) on the pipe-end. Calculate Q with and without the losses in the termination. If the Q-change in < 1% this is also a good position for testing a cavity

- Transit-time factor (TTF): The TTF gives the effective acceleration for a particle crossing an acceleration gap. This value is less than 1 due to the time-variation of the field during the particle crossing. Some codes have automatic or manual procedures to calculate the TTF. The literature mostly provides approximations of the proper integrals for specific configurations.
- If you cannot confirm their assumptions (like z=0 @ center of gap,) use the general expressions provided in the first class.

- <u>Tuning sensitivities:</u> Frequency changes from small changes in geometry need to be determined. Those might not be very accurate, as the discretization errors can dominate the solutions. Some solutions:
 - Model a few larger changes, check if the sensitivity behaves linear
 - Use expert system meshers, those for small changes in geometry only move element nodes to new positions without remeshing
 - Use Slater's Perturbation Theorem (also useful for LFD and surface removal)

$$\frac{\Delta \omega}{\omega} = \frac{\int_{\Delta V} (\mu_0 H^2 - \epsilon_0 E^2) dV}{\int_{\Delta V} (\mu_0 H^2 + \epsilon_0 E^2) dV} = \frac{\Delta U_m - \Delta U_e}{U}$$

- Dealing with small changes in geometry: A typical situation is the determination of the external Q (coupling) for a coupler attached to a resonator. To avoid errors due to the change in discretization the following strategy works well:
 - Model different positions of a substructure simultaneously,
 only changing material properties, this preserves meshing



■ Warning on R/Q calculation: There are two different conventions on this quantity in use: The "circuit" convention and the "linac" convention. They differ by a factor of 0.5. Make sure what convention your code is using:

$$R/Q=V^2/(\omega U)$$
 or $R/Q=V^2/(2\omega U)$

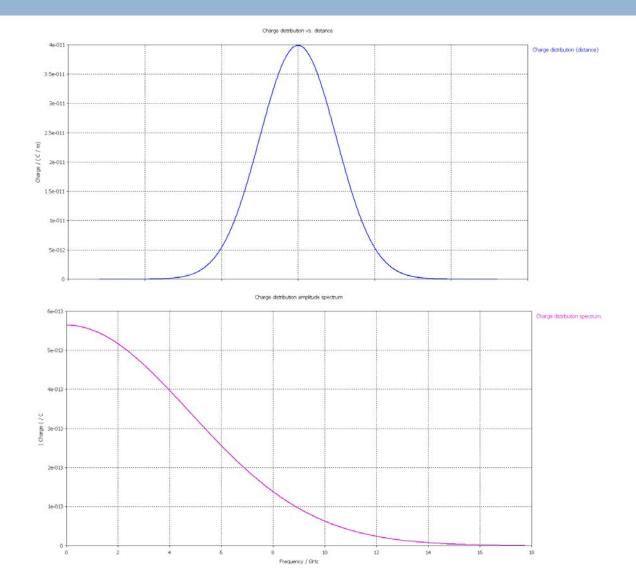
Location of solutions: If you export solutions for further processing, make sure you know about proper allocation. Solutions can be allocated along element edge, in the center of an element or on the end points of element edges

- Meshing: Many codes use auto mesh generators that fulfill certain criteria. For those who do not provide automeshing or for control of special circumstances some rules should be kept in mind:
 - Consider the highest frequency relevant for a simulation and make sure that your mesh uses at least 10 steps per wavelength at this frequency.
 - For the typically low operation frequency problem can be made small, keep in mind that calculation of HOMs increases the required density
 - For interaction with particles, especially for wake fields of ultrashort bunches, meshing needs to extremely fine (e.g. for a bunchlength of 1mm (rms) the highest bunch frequency is 177 GHz)
 - PIC codes often require equidistant meshes

■ Meshing:

Bunch of 10mm length rms

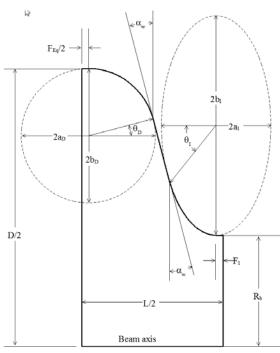
Spectrum extends to 18 GHz



Auto-generation of elliptical resonators:

■ Their outline is a complex polygon made up from straight, circular and elliptical segments.

- Optimization is made hard by the fact that the segment transitions need to be smooth.
- This is addressed in several codes that integrated parametric descriptions for elliptical resonators for optimization.
- Superfish and Buildcav (a wrapper on top of Superfish) also include assembly of separately designed mid and end-cells of a multi-cell cavity



The End

Thanks to the community from which I borrowed examples and illustrations

As I do not credit any providers, please refrain from using these materials outside this meeting

I can provide references for specific topics if needed